

Quick Start User Guide: TROPES CrIS Ozone Level 2 Standard and Summary Data Product Files

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1 Introduction

1.1 Overview and Document Scope

This document is to be used as a Quick start user guide for using the TROPES CrIS Ozone Level 2 Standard Product Files.

1.2 Dataset Description

This user guide describes the TROPES CrIS Level 2 Standard product files for ozone (O₃).

Product Information	Description
Parameters	O ₃ profile
Data Product Provenance	MUSES Version 1.10
Approximate file size	30 MB
Spatial coverage	Regular collections have global coverage: Nominal latitude range: 70 N to 50 S Nominal longitude range: -180 to 180 Special collections: Spatial coverage varies by collection
Temporal coverage	Each L2 nominal Standard file contains 1 day of data
File format	netcdf
Vertical sensitivity	The ozone profiles typically have sensitivity between approximately 800 hPa and the upper stratosphere. There is sensitivity in the retrievals to ozone in the troposphere, often around 0.8-1.2 degrees of freedom
Data quality	The data have undergone a pre-quality check, which involves checks for retrieval convergence. There are no checks for clouds or land versus ocean as we do not find these to substantively affect the quality of the retrieval as long as the retrieval has converged. The ozone data has undergone some preliminary validation compared to ozonesondes, with a much more thorough evaluation currently underway
Uncertainty	Uncertainties on vertically-averaged ozone values between 825.4 and 10 hPa are estimated to vary between 0.2-0.9 ppb for a single sounding.
Validation Stage	Stage 2 according to NASA guidelines https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels
Retrieval Levels	26 levels: from surface to top-of-atmosphere
FillValues	-999

1.3 Filename

The Standard Products adhere to the following filename convention:

```
[TROPES]_[File  
type]_[Instrument]_[Parameter]_[version]_[Date or  
label].nc
```

Example:

```
TROPES_CrIS-  
SNPP_L2_Standard_O3_20200912_MUSES_R1p9_SC_F0p1.nc
```

2 Product File Contents and Parameter Description

2.1 Variables listed in the Standard Product

Please see the README for a list of variables included in the Level 2 Standard product file.

3 References

The following references were also used in the development of this documentation:

1. Fu, D. et al., Retrievals of tropospheric ozone profiles from the synergism of AIRS and OMI: methodology and validation, *Atmos. Meas. Tech.*, doi:10.5194/amt-11-5587-2018, 2018.
2. Fu, D. et al., Characterization of ozone profiles derived from Aura TES and OMI radiances, *Atmospheric Chemistry and Physics*, doi:10.5194/acp-13-3445-2013, 2013.
3. Boxe, C.S., et al., Validation of northern latitude Tropospheric Emission Spectrometer stare ozone profiles with ARC-IONS sondes during ARCTAS: sensitivity, bias and error analysis, *Atmospheric Chemistry and Physics*, doi:10.5194/acp-10-9901-2010, 2010.
4. Nassar, R., Logan, J. A., Worden, H. M., et al.: Validation of Tropospheric Emission Spectrometer (TES) nadir ozone profiles using ozonesonde measurements, *J. Geophys. Res.*, 113, D15S17, doi:10.1029/2007JD008819, 2008.
5. Worden, H. M. et al., Comparisons of Tropospheric Emission Spectrometer (TES) ozone profiles to ozonesondes: Methods and initial results, *J. Geophys. Res.*, 112, D03309, doi:10.1029/2006JD007258, 2007.
6. Bowman, K.W. et al., Tropospheric Emission Spectrometer: Retrieval Method and Error Analysis, *IEEE Trans. Geosci. Remote Sensing*, 44, 1297- 1307, 2006.
7. Worden, H. M. et al., Predicted errors of tropospheric emission spectrometer nadir retrievals from spectral window selection, *J. Geophys. Res.*, 109, D09308, doi:10.1029/2004JD004522, 2004.
8. Rodgers, C. D., and B. J. Connor (2003), Intercomparisons of remote sounding instruments, *J. Geophys. Res.*, 108(D3), 4116, doi:[10.1029/2002JD002299](https://doi.org/10.1029/2002JD002299)

4 Extended User Guide: L2 Standard Product

This extended user guide shows how to compare these ozone data products to ozonesonde, aircraft or model fields and calculate uncertainties.

4.1 How to compare to ozonesonde data

All comparisons between remotely sensed data and *in situ* measurements or high resolution model fields must account for the sensitivity of the remotely sensed measurement and any regularization used with the remotely sensed measurements. Otherwise errors will be incurred with the comparisons. The validation technique of comparing retrievals of ozone from satellites to ozonesondes has been demonstrated many times, most recently by Fu et al., 2018 for ozone derived from joint Atmospheric Infrared Sounder/Ozone Monitoring Instrument (AIRS/OMI) retrievals and Boxe et al., 2010 for ozone retrieved by the Tropospheric Emission Spectrometer (TES).

Here is the general approach for comparison of the TROPES data to models or vertical profile measurements such as from aircraft:

- 1) Construct the O₃ profile using the model or aircraft fields (for the purpose of this demonstration we will call this \mathbf{x}_{true}).
- 2) Construct the observation operator as the following :

$$\mathbf{H}(\cdot) = \ln(\mathbf{x}_a) + \mathbf{A}(\ln(\cdot) - \ln(\mathbf{x}_a))$$
- 3) Apply observation operator to the O₃ profile:

$$\hat{\mathbf{x}} = \exp[\mathbf{H}(\mathbf{x}_{true})]$$

In the netcdf product file and in the equation, \mathbf{x}_a is the constraint vector used to regularize the retrieval. $\mathbf{H}(\cdot)$ is the observation operator, where the (\cdot) represents a model or *in situ* profile. \mathbf{A} is the averaging kernel matrix and must be matrix multiplied by $\ln(\mathbf{x}_{true}) - \ln(\mathbf{x}_a)$. After this operation one can compare the modified O₃ profile ($\hat{\mathbf{x}}$) to the retrieved “x” variable in the netcdf product file. Note that the averaging kernel matrix (\mathbf{A}) is not symmetric, so getting the row/column order of \mathbf{A} correct is critical. You can check your work by using the above equation with the zeroth entries for the averaging kernel, \mathbf{x}_a and using the zeroth entry for \mathbf{x} as \mathbf{x}_{true} . If your test operation (steps 1-3) matches the variable \mathbf{x}_{test} then the operation is correct.

4.2 Validation Summary

Summary Statement: Based on the NASA Validation Guidelines (see link in Table 1), we determined that the TROPES L2 Standard CO products are at Validation Stage 1.

Preliminary validation analysis of TROPES/CrIS ozone retrievals are underway using comparisons to ozone. A full validation analysis will be provided in a publication expected in the second half of 2021.

Figure 1 shows daily comparisons for ozone profiles from CrIS to ozonesondes. The comparisons are for data near Madrid, Spain on May 6, 2020 and Tsukuba, Japan on April 30, 2020. The figure shows the percentage difference, $((\text{sonde}-\text{satellite})/\text{sonde})$ as a function of pressure. The solid red line is the mean of all the comparisons for that day, with dashed red lines showing the mean value \pm the standard deviation. The blue profiles are the individual differences for that day. Both sites show that in the troposphere, CrIS is biased high with the bias switching over near the tropopause and becoming a positive bias in the stratosphere (not shown).

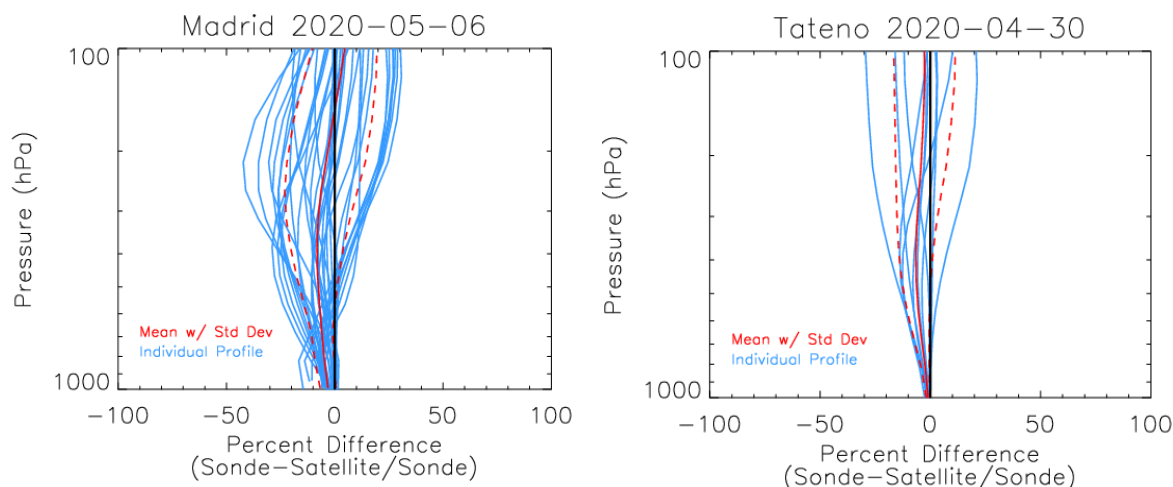


Figure 1. Profile comparisons of CrIS ozone to ozonesondes. On the left are 32 profile comparisons shown a percentage difference with a single sonde (blue lines). The mean difference is the solid red line and mean \pm the standard deviation is the red dashed lines. On the right is a similar plot for Tsukuba (Tateno), Japan. Both show the satellite data to be on average biased high relative to the sonde in the troposphere.

Figure 2 is a time series of CrIS ozone, this time a middle tropospheric mean value (between 300 and 750 hPa) compared to the corresponding sonde value. This time the difference is the absolute difference (bias), sonde value minus the satellite value. The data is from 2018 with the Madrid and Tsukuba time series shown. The data show the daily mean bias and standard deviation. There is some seasonal variability in the data but the Madrid comparison does show that the CrIS data is biased high in most cases. The bias is less clear in the Japan data, but there are also many fewer comparisons for that site. These preliminary checks of the data show a high bias in the troposphere at several other sites, including one in the Southern hemisphere, during 2018.

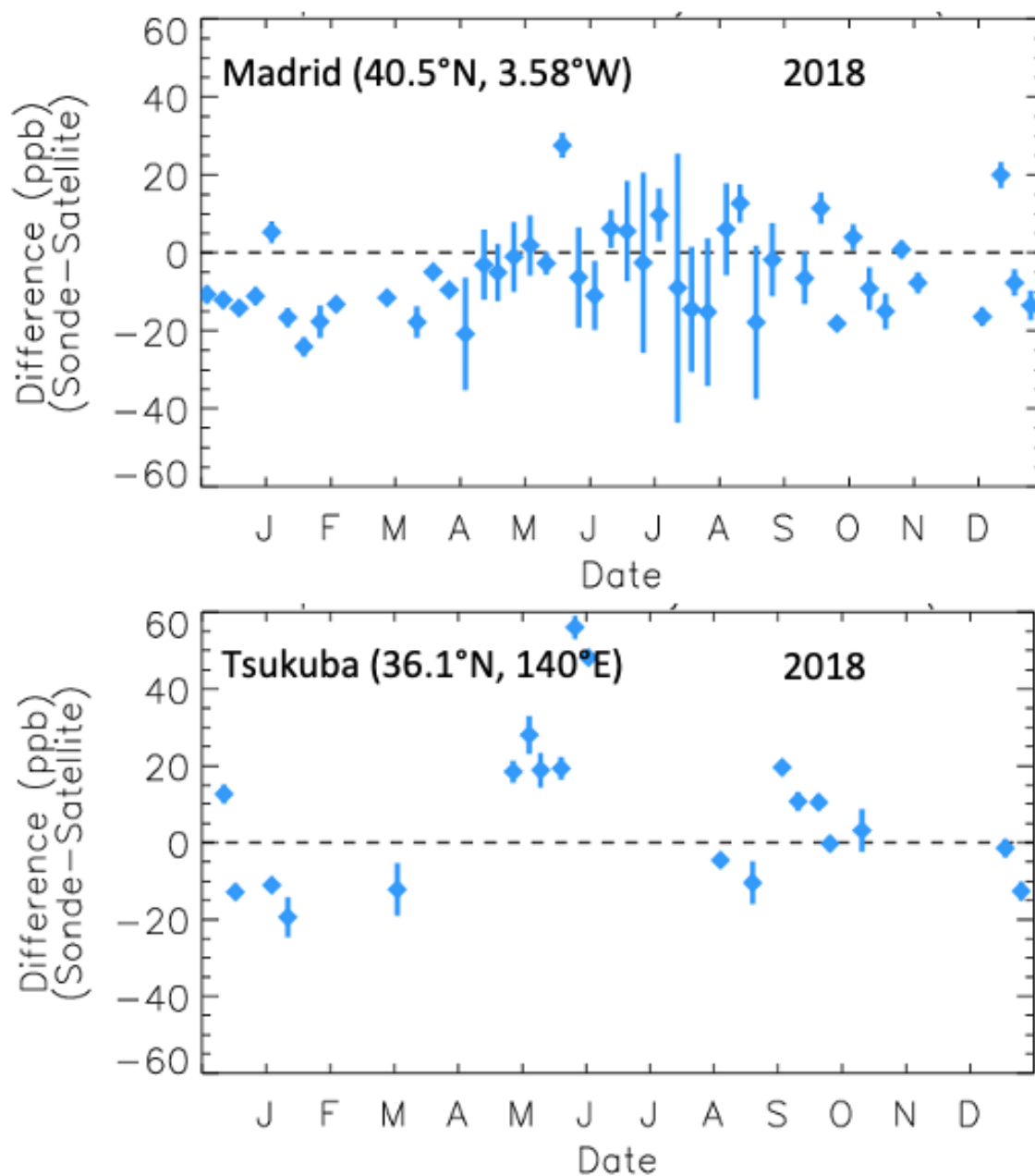


Figure 2. Time series of the mid-tropospheric mean value difference between the CrIS and the ozonesonde data (sonde-CrIS). Mean value between 750 and 300 hPa is shown for Madrid (top) and Tsukuba (bottom) for 2018.

Appendix A. Retrieval levels

The table below contains the nominal retrieval levels. For each sounding, the surface pressure level is inserted into the retrieval levels set. Any retrieval levels below the surface pressure level are omitted.

Index	Pressure [hPa]
1	1211.53
2	1000.00
3	825.402
4	681.291
5	562.342
6	464.16
7	383.117
8	316.227
9	261.016
10	215.444
11	161.561
12	121.152
13	90.8518
14	68.1295
15	51.0896
16	38.3119
17	28.7299
18	21.5443
19	16.1560
20	12.1153
21	9.08514
22	6.81291
23	4.64160
24	1.61560
25	0.681292
26	0.10000

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